AFRL-RW-EG-TR-2015-108

Stochastic Estimation via Polynomial Chaos

Douglas V. Nance

Air Force Research Laboratory
Munitions Directorate/Ordnance Division
Lethality, Vulnerability and Survivability Branch
(AFRL/RWML)
Eglin AFB, FL 32542-5910

October 2015

Interim Report

AIR FORCE RESEARCH LABORATORY
MUNITIONS DIRECTORATE

■ **Air Force Materiel Command** ■ **United States Air Force** ■ **Eglin Air Force Base, FL 32542**

NOTICE AND SIGNATURE PAGE

This report was cleared for public release by the 96th Air Base Wing, Public Affairs Office, and is available to the general public, including foreign nationals. Copies may be obtained from the Defense Technical Information Center (DTIC) < http://www.dtic.mil/dtic/index/html>.

AFRL-RW-EG-TR-2015-108 HAS BEEN REVIEWED AND IS APPROVED FOR PUBLICATION IN ACCORDANCE WITH ASSIGNED DISTRIBUTION STATEMENT.

FOR THE DIRECTOR:

HOWARD G. WHITE, PhD   KIRK J. VANDEN, PhD
Chief Engineer   Technical Advisor
Ordnance Division   Lethality, Vulnerability and Survivability Branch

PEDRO LOPEZ-FERNANDEZ
Program Manager
Lethality, Vulnerability and Survivability Branch

This report is published in the interest of scientific and technical information exchange, and its publication does not constitute the Government's approval or disapproval of its ideas or findings.

Distribution A

This page intentionally left blank

1. REPORT DATE *(DD-MM-YYYY)* xx-10-2015	2. REPORT TYPE Interim		3. DATES COVERED *(From - To)* 20-04-2015 – 07-08-2015	
4. TITLE AND SUBTITLE Stochastic Estimation via Polynomial Chaos			5a. CONTRACT NUMBER	
			5b. GRANT NUMBER	
			5c. PROGRAM ELEMENT NUMBER 62602F	
6. AUTHOR(S) Douglas V. Nance			5d. PROJECT NUMBER 25024504	
			5e. TASK NUMBER	
			5f. WORK UNIT NUMBER W0TP	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Air Force Research Laboratory, Munitions Directorate Ordnance Division Lethality, Vulnerability, and Survivability Branch (AFRL/RWML) Eglin AFB FL 32542-6810			8. PERFORMING ORGANIZATION REPORT NUMBER AFRL-RW-EG-TR-2015-108	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Research Laboratory, Munitions Directorate Ordnance Division Lethality, Vulnerability, and Survivability Branch (AFRL/RWML) Eglin AFB FL 32542-6810 Technical Advisor: Kirk J. Vanden, PhD			10. SPONSOR/MONITOR'S ACRONYM(S)	
			11. SPONSOR/MONITOR'S REPORT AFRL-RW-EG-TR-2015-108	
12. DISTRIBUTION / AVAILABILITY STATEMENT Distribution A: Approved for public release; distribution unlimited. Approval Confirmation 96W-2015-0348, dated 03 December 2015				
13. SUPPLEMENTARY NOTES				

14. ABSTRACT
This expository report discusses fundamental aspects of the polynomial chaos method for representing the properties of second order stochastic processes. As originally developed by Norbert Weiner, a polynomial chaos represents key properties of a stochastic process through the application of finite series of orthogonal polynomials. The attendant polynomial expansion is used to describe the statistical properties of a stochastic process based upon an input uncertainty. The statistics of a random process is given by evaluating the appropriate polynomial chaos for an input uncertainty represented by one or more random variables. An evolved application of this idea applies a polynomial chaos to represent uncertainties in boundary or initial conditions for partial differential equations. Here, the elementary theory of the polynomial chaos is presented followed by the details of a number of example calculations where the statistical mean and standard deviation are compared against exact solutions. The Legendre chaos is described in some detail for uniformly distributed input random variables. Also, the Hermite chaos is discussed.

15. SUBJECT TERMS
stochastic process, random variables, polynomial chaos, Legendre polynomials, Hermite polynomials, statistics, Cameron-Martin theorem, Karhunen-Loeve expansion, uncertainty quantification

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Douglas V. Nance
a. REPORT UNCLASSIFIED	b. ABSTRACT UNCLASSIFIED	c. THIS PAGE UNCLASSIFIED	SAR	53	19b. TELEPHONE NUMBER *(include area code)*

Distribution A

This page intentionally left blank

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

1.0 SUMMARY

This expository report discusses fundamental aspects of the polynomial chaos method for representing the properties of second order stochastic processes. As originally developed by Norbert Weiner, a polynomial chaos represents key properties of a stochastic process through the application of finite series of orthogonal polynomials. The attendant polynomial expansion is used to describe the statistical properties of a stochastic process based upon an input uncertainty. The statistics of a random process is given by evaluating the appropriate polynomial chaos for an input uncertainty represented by one or more random variables. An evolved application of this idea applies a polynomial chaos to represent uncertainties in boundary or initial conditions for partial differential equations. Here, the elementary theory of the polynomial chaos is presented followed by the details of a number of example calculations where the statistical mean and standard deviation are compared against exact solutions. The Legendre chaos is described in some detail for uniformly distributed input random variables. Also, the Hermite chaos is discussed for random variables possessing a Gaussian distribution. A number of example problems are solved.

2.0 INTRODUCTION

Real world problems involving science and engineering always involve uncertainty. Specific uncertainties in the form of imprecisely known input parameters propagate through a physical mechanism and create uncertainty in the system output forming a stochastic process involving one or more random variables. A simple example considered later in this report addresses the oblique shock wave formed by the supersonic flow over a wedge. In this scenario, we presume that the wedge angle, with respect to the freestream direction, is imprecisely known. The wedge angle is regarded as a random variable with a mean value and a standard deviation based upon a distribution. The ensuing oblique shock wave angle becomes a function of this random variable and takes on a randomness that can be assessed by the polynomial chaos. Other properties associated with the shocked flow field also adopt random properties that may also be assessed by the chaos. This example is conceptually simple to understand, but the same idea can be extended to other more complicated physical systems. The solutions of either ordinary or partial differential equations subject to uncertainties in initial or boundary conditions also inherit random characteristics that can be revealed by the chaos. For this reason, there are many applications for this mathematical tool. Before beginning a detailed mathematical development of the chaos, it is instructive to discuss the nature of physical uncertainties.

2.1 The Concept of Uncertainty

As is the case for physical properties, the concept of uncertainty has been analyzed and properly defined.[1] Consider the uncertainty existing in the measurement or calculation of a physical quantity. If the quantity possesses a true value with no variation, then the variation sensed in measuring or calculating the quantity is referred to epistemic. On the other hand, if a physical quantity exhibits a natural variability, (that is, it possesses no true (or certain) value), then the associated uncertainty is denoted as aleatoric. In the Bayesian probabilistic framework, epistemic uncertainties can be addressed by techniques such as those described below. Aleatoric uncertainties are readily treated by probabilistic methods. The primary application considered in the results section of this report can be regarded as having epistemic uncertainty. In this case, the wedge angle is assumed to possess a small variation. With the use of clever mathematical techniques, the statistical parameters (e.g., mean and standard deviation) of functions of these uncertainties can be predicted with accuracy.

2.2 Mathematical Representation of Stochastic Processes

The mathematical development of stochastic processes is extensive, the culmination of decades of research, so only the briefest description is provided here. The first requisite concept is that of the sample space. A sample space is the set of all possible outcomes of an experiment whether the experiment is simple such as a coin toss or complex, or the measurement of temperature or fluid stress taken at some point in a turbulent flow field. Detailed examples of sample spaces are contained in Ross.[2] On a given sample space, much like a mathematical domain, we define functions denoted as random variables. For example, on the event space for a coin toss, we can define a random variable that counts the number of heads occurring for a certain number of coin tosses. As another example, we may define a random variable that represents the time varying electrical voltage existing at a point in an electronic circuit. The

former is a discrete random variable while the latter is a continuous random variable. A discrete random variable takes on either a finite or countably infinite number of values while the continuous random variable takes on a finite number of values. Building upon these concepts, a stochastic process is a collection of random variables $X(t)$ indexed by a set T where $t \in T$. T is denoted as the indexing set; it may consist of either a finite or infinite number of elements depending on the nature of the stochastic process. More specifically, $X(t)$ is the state of the stochastic process X at time t.[2] In the context of this report, $X(t)$ may be regarded as the uncertainty in some quantity. With this assertion, we may envision functions of the uncertainty represented by $X(t)$. This function of the uncertainty (random variable) requires the use of "functionals"; a functional may be thought of as a function of functions.[3] In this sense, a functional is defined on a vector space of functions, and this concept represents a significant mathematical abstraction beyond that of the more commonly known vectors defined in Euclidean space $\Re^n$.

A significant difficulty in simulating stochastic processes, or more particularly, in simulating stochastic variation in otherwise deterministic systems lies in the lack of an intuitive understanding of function spaces.[4] For stochastic problems, the function space must be "measurable" with respect to a probability space consisting of the sample (or event) space, a σ-algebra defined on the event space and a probability measure P. The σ-algebra is a collection of subsets of the event space that possess special properties.[5] One approach to the problem of simulating random or stochastic processes is Monte Carlo simulation, a technique that requires the repeated sampling of the σ-algebra. This method, although highly effective, requires sampling many, many points requiring a great deal of computing resources.[6,7,8] Another approach that can be less resource intensive entails representing the stochastic process in terms of a set of orthogonal functions defined on the function space.[4,5] Although the resulting orthogonal decomposition (a spectral approach) consists of an infinite series, the series can be finitely truncated for computational purposes. The principal function space containing the orthogonal function set is denoted as $L_2(\Omega, P)$ where Ω is the sample space, and P is the probability measure. L_2 is a Hilbert space known as the space of square integrable functions widely applied throughout mathematical physics.[9] For a given stochastic process defined at points in space, an orthogonal decomposition of great theoretical interest is the Karhunen-Loeve expansion.[4,5]

The Karhunen-Loeve expansion provides an orthogonal decomposition for any second order random field (stochastic process) $w(\vec{x}, \omega)$ where $\vec{x}$ is the space coordinate and θ is an element of the random event space. The Karhunen-Loeve expansion for this random process is written as

$$w(\vec{x}, \omega) = \overline{w}(\vec{x}) + \sum_{n=0}^{\infty} \xi_n(\omega) \sqrt{\lambda_n} \, f_n(\vec{x}) \tag{1}$$

where $\xi_n(\omega)$ is a set of random variables defined on the event space Ω, and $f_n(\vec{x})$ is a set of deterministic orthogonal functions. It can be shown that the orthogonal function set consists of the eigenfunctions for the covariance function of the random process. The λ_n are the associated eigenvalues.[4,5] The space-dependent mean value for the random process is $\overline{w}(\vec{x})$. As defined,

this expansion is convergent in mean squared error and is unique, but it is mostly of theoretical interest. It is not very useful for practical computations since the covariance function for the random process must be known *a priori* in order to guarantee the expansion's convergence and uniqueness.[4] In most cases, the covariance function is unknown. Still, the expansion motivates the search for other orthogonal decompositions that are more easily applied even if the convergence of individual decompositions must be carefully monitored. The method showcased in this report applies a polynomial chaos expansion to construct the orthogonal decomposition. An early example of this expansion is Weiner's homogeneous chaos.[10]

Wiener's continuous homogeneous chaos cast in three dimensions is a measurable function ρ with

$$\rho = \rho(x_1, x_2, x_3; \beta) \tag{2}$$

In this chaos, $\vec{x} = (x_1, x_2, x_3)$ is the deterministic space point while $\beta \in [0,1]$ represents the random range of the stochastic process. Other chaos formulations have been proposed and implemented. A specific chaos is due to Cameron and Martin and is denoted as a Fourier-Hermite chaos for a chosen functional. The Cameron-Martin theorem states that the Fourier-Hermite series of any real or complex functional $F[x]$ in L_2 converges to $F[x]$ in the L_2 sense with Wiener measure.[3] In the same reference, the orthogonality of the Fourier-Hermite chaos is also demonstrated. The measure (or weighting function) used in integration is the same as the probability density function for Gaussian random variables.[11] This chaos is still widely applied for uncertainties consisting of Gaussian random variables. To provide for the assessment of other types of random variables, other chaos formulations have been developed. These formulations are included in the generalized polynomial chaos or "Askey Scheme".[11] In this generalized chaos, an appropriate set of orthogonal polynomials is paired with a random variable distribution. As described in Reference [11,12,13], these combinations are shown in Table 1.

Table 1. Distribution Function/Orthogonal Polynomial Chaos Combinations

Distribution Function	Orthogonal Polynomial Set
Gaussian	Hermite
Uniform	Legendre
Gamma	Laguerre
Beta	Jacobi
Poisson	Charlier
Negative Binomial	Meixner
Binomial	Krawtchouk
Hypergeometric	Hahn

Consider a Hermite chaos for random function α formulated for exactly one random variable ξ defined for the event space Ω (where $\omega \in \Omega$). For this scenario, the chaos expansion is written as

Distribution A

$$\alpha(\xi(\omega)) = \sum_{n=0}^{\infty} \alpha_n H_n(\xi(\omega)) \tag{3}$$

The form of this expansion is quite simple since there are no space or time parameters explicitly associated with the random function. In this sense, this problem is analogous to a single coin toss or dice throw problem. Specifically, the α_n are expansion coefficients that are determined to complete the representation of the random function α. The notation H_n represents the order n Hermite polynomial where $n = 0, 1, 2 \ldots$. The Hermite polynomials are written as functions of the random variable ξ, e.g., $H_0(\xi) = 1$; $H_1(\xi) = \xi$; $H_2(\xi) = \xi^2 - 1$, etc.[4] If the random function involves more than one random variable, e.g., ξ_1 and ξ_2, then the expansion functions are formed by tensor products of the polynomials cast in one random variable. The procedure for determining the expansion coefficients α_n is explained in the following section of this report.

Distribution A

3.0 METHODS, ASSUMPTIONS AND PROCEDURES

In the discussions below, we develop the equations needed in applying a polynomial chaos to represent uncertainties in stochastic processes. The two principal approaches for applying a polynomial chaos are (i) the intrusive method and (ii) the non-intrusive method. Although this report concentrates on the non-intrusive application, the intrusive approach is also briefly described. For the example problems shown in Section 3, detailed equations are presented for the Legendre polynomial chaos associated with for a system of uniform random variables. Due to the simplicity of the probability measure for the uniform random variable, this chaos is the easiest to derive. As a result, the development presented below is intended to be pedagogical. As a second discussion, the Hermite polynomial chaos is developed for Gaussian random variables.

3.1 Intrusive Polynomial Chaos

This manifestation of polynomial chaos is denoted intrusive since it entails alterations to the system of governing equations. An example discussed in the literature involves solution of the incompressible Navier-Stokes equations.[1,17] In this case, a single parameter is decomposed say, u, the x-velocity component.

$$u(\vec{x}, t = 0) = \bar{u}(\vec{x}) + \xi \, \hat{u}(\vec{x}) \tag{4}$$

In this expression, ξ is a random variable with unit variance. Polynomial chaos expressions for all stochastic quantities, e.g.,

$$u(\vec{x}, t, \xi) = \sum_{k=0}^{P} u_k(\vec{x}, t) \, \Psi_k(\xi) \tag{5}$$

Expressions such (5) are substituted into the Navier-Stokes equation. By use of the Galerkin procedure, evolution equations for expansion coefficients u_k may be derived.[17] For instance,

$$\frac{\partial u_k}{\partial t} + \sum_{i=0}^{P} \sum_{j=0}^{P} M_{ijk} (u \bullet \nabla) u = -\nabla p_k + \nu \nabla^2 u_k \tag{6}$$

$$\nabla \bullet u_k = 0 \tag{7}$$

for $k = 0, \ldots, P$, and

$$M_{ijk} = \frac{\langle \Psi_i \Psi_j \Psi_k \rangle}{\langle \Psi_k^2 \rangle} \tag{8}$$

The M_{ijk} are convolution integrals rendering numbers for use in (6). Equations (6) and (7) must be solved via numerical means to obtain the expansion coefficients. This alteration of the

governing equations is characteristic of intrusive polynomial chaos methods. Given the difficulty associated with implementing these schemes, implementation details are not provided here.

3.2 Fundamentals of Polynomial Chaos

As its most basic idea, a polynomial chaos expands the uncertainty of a stochastic process in terms of a system of orthogonal polynomials. By increasing the number of terms in the expansion, the overall accuracy of the method is enhanced. Of course, obtaining the expansion coefficients for the series constitutes the majority of the labor required to implement this method. The polynomial chaos approach applied here is a direct application of the equation

$$\alpha^*(\vec{x}, t, \vec{\xi}) = \sum_{j=0}^{\infty} \alpha_j(\vec{x}, t)\, \Psi_j(\vec{\xi}) \tag{9}$$

where $\alpha^*(\vec{x}, t, \vec{\xi})$ is the random process of interest; Ψ_j is an element of an orthogonal family of polynomials, and the $\alpha_j(\vec{x}, t)$ are the expansion coefficients for these polynomials. Of course, $\vec{\xi}$ is a vector of random variables representing the system's uncertainties. Each of these random variables is usually chosen as of either "standard" uniform or Gaussian form. Of course, other types of random variables can be used. The usual procedure is to have the random variable match the random characteristics of the uncertainty. $\Psi_j(\vec{\xi})$ is a multi-dimensional orthogonal polynomial in that

$$\int_{D(\vec{\xi})} \Psi_j \Psi_k\, dw(\vec{\xi}) = \left\langle \Psi_j^2 \right\rangle \delta_{jk} \tag{10}$$

Equation (10) is the statement of orthogonality. The expected value for α^* may be computed as follows. The expected value is defined as $\left\langle \alpha^* \right\rangle$; therefore, by truncating the series to a finite number of terms,

$$\left\langle \alpha^*(\vec{x}, t) \right\rangle = \sum_{j=0}^{P} \alpha_j(\vec{x}, t) \int_{D(\vec{\xi})} \Psi_j(\vec{\xi})\, w(\vec{\xi})\, d\vec{\xi} \tag{11}$$

$$\left\langle \alpha^*(\vec{x}, t) \right\rangle = \alpha_0(\vec{x}, t) \int_{D(\vec{\xi})} \Psi_0(\vec{\xi})\, w(\vec{\xi})\, d\vec{\xi} + \sum_{j=1}^{P} \alpha_j(\vec{x}, t) \int_{D(\vec{\xi})} \Psi_j(\vec{\xi})\, w(\vec{\xi})\, d\vec{\xi} \tag{12}$$

Although series truncation is common practice, it must be performed carefully since it may affect series convergence. Equation (12) may be simplified that realizing that Ψ_0 is the zeroth order polynomial, a constant, so it can be chosen as unity. Thus,

$$\left\langle \alpha^*(\vec{x}, t) \right\rangle = \alpha_0(\vec{x}, t) \int_{D(\vec{\xi})} w(\vec{\xi}) \, d\vec{\xi} + \sum_{j=1}^{P} \frac{\alpha_j(\vec{x}, t)}{\Psi_0} \int_{D(\vec{\xi})} \Psi_0 \cdot \Psi_j(\vec{\xi}) \, w(\vec{\xi}) \, d\vec{\xi} \tag{13}$$

In equation (13), the first term is evaluated by noting that the probability measure is written as

$$dw(\vec{\xi}) = w(\vec{\xi}) \, d\vec{\xi} \tag{14}$$

Applying the rules of probability,

$$\int_{D(\vec{\xi})} w(\vec{\xi}) \, d\vec{\xi} = 1 \tag{15}$$

Next, observe that the second term contains the rewritten integral

$$\int_{D(\vec{\xi})} \Psi_0 \cdot \Psi_j(\vec{\xi}) \, w(\vec{\xi}) \, d\vec{\xi} \,, \quad j = 1, 2, \ldots, P \tag{16}$$

The rewrite is made possible since Ψ_0 is a constant, equal unity. By using (10) and (15), the integral in (16) is zero. Hence,

$$\left\langle \alpha^*(\vec{x}, t) \right\rangle = \alpha_0(\vec{x}, t) \tag{17}$$

The variance can be computed by a similar set of arguments. Recall that

$$\mathrm{var}(\alpha^*) = \left\langle \alpha^{*2} \right\rangle - \left\langle \alpha^* \right\rangle^2 \tag{18}$$

The first term in (18) is evaluated by substituting (9), i.e.,

$$\left\langle \alpha^{*2} \right\rangle = \left\langle \sum_{j=0}^{P} \alpha_j \Psi_j(\vec{\xi}) \cdot \sum_{k=0}^{P} \alpha_k \Psi_k(\vec{\xi}) \right\rangle = \left\langle \sum_{j=0}^{P} \sum_{k=0}^{P} \alpha_j \, \alpha_k \Psi_j(\vec{\xi}) \Psi_k(\vec{\xi}) \right\rangle \tag{19}$$

By using the integral to compute the expectation,

$$\left\langle \alpha^{*2} \right\rangle = \sum_{j=0}^{P} \sum_{k=0}^{P} \alpha_j \, \alpha_k \int_{D(\vec{\xi})} \Psi_j \Psi_k \, w(\vec{\xi}) d\vec{\xi} \tag{20}$$

Applying (10), we obtain

$$\left\langle \alpha^{*2} \right\rangle = \sum_{j=0}^{P} \sum_{k=0}^{P} \alpha_j \, \alpha_k \left\langle \Psi_k^2 \right\rangle \delta_{jk} = \sum_{j=0}^{P} \alpha_j^2 \left\langle \Psi_j^2 \right\rangle \tag{21}$$

Distribution A

Substituting (21) and (17) into (18), we have that

$$\text{var}(\alpha^*(\vec{x},t)) = \sum_{j=0}^{P} \alpha_j^2(\vec{x},t)\langle \Psi_j^2 \rangle - \alpha_0^2(\vec{x},t) = \sum_{j=1}^{P} \alpha_j^2(\vec{x},t)\langle \Psi_j^2 \rangle \qquad (22)$$

The standard deviation $\sigma(\vec{x},t)$ is, by definition, the square root of the variance, so

$$\sigma(\vec{x},t) = \text{var}(\alpha^*(\vec{x},t)) = \sqrt{\sum_{j=1}^{P} \alpha_j^2(\vec{x},t)\langle \Psi_j^2 \rangle} \qquad (23)$$

As illustrated by (17) and (23), the mean and standard deviation for the random process are easily calculated from the polynomial chaos expansion.

3.3 Point Collocation Non-Intrusive Polynomial Chaos

Non-intrusive polynomial chaos methods do not require modification of the governing equations. Of equal importance is the fact that there is more than one non-intrusive method. Spectral progression and linear regression are two such methods.[18] As with the intrusive method, equation (9) is applied to physical properties of interest say, absolute pressure for a fluid dynamics problem. The property of interest is represented by $\alpha^*(\vec{x}, t, \vec{\xi})$. It is important to realize that $\vec{\xi}$ represents the input or driving uncertainty say, a varying initial or boundary condition. For the point collocation method, the random variable $\vec{\xi}$ is randomly sampled in accordance with its statistical distribution. Each sample forms a realization of the random process α^*. For a direct determination of the polynomial chaos coefficients α_j, $P+1$ samples, $\vec{\xi}_j$, $j = 0,1,\ldots,P$, of the random process α^* are computed (perhaps by use of fluid dynamics computer codes for each $\vec{\xi}_j$). Applying this idea prior to series truncation, equation (9) is rewritten as

$$\alpha^*(\vec{x}, t, \vec{\xi}_j) = \sum_{k=0}^{\infty} \alpha_k(\vec{x}, t)\, \Psi_k(\vec{\xi}_j), \quad j = 0,1,\ldots,P \qquad (24)$$

The polynomials $\Psi_k(\vec{\xi}_j)$ are calculated for the choice of ξ_j, so these parameters are known quantities. Equation (24) actually represents a system of $P+1$ equations in $P+1$ unknowns. As a system of linear equations, (24) can be solved for the α_k. The example problems documented later in this report apply LU-decomposition with partial pivoting to solve this equation.[19] Naturally, the title of this method arises from the use of the collocation points $\vec{\xi}_j$.

The point collocation method applied here is introduced in References 14, 15, 20 and 21. It is relatively easy to implement, yet it is subject to some limitations that must be mentioned. Recall from the preceding paragraph that the polynomial chaos equations are defined at the $P+1$

collocation points. For a given continuous random variable distribution (e.g., uniform, beta, Gaussian), a random selection of collocation points is not unique. For this reason, the computed mean, standard deviation and other statistical parameters are not unique. A number of numerical techniques have been designed as remedies for this difficulty. One approach is to generate a more even point distribution to provide better coverage of the collocation point space. This may be accomplished through the use of Hammersley or Halton data sets.[22,23] Numerical experiments conducted by the author demonstrate that a Hammersley point set does provide better coverage of the uncertainty distribution. Unfortunately, the lack of true randomness in this data set tends to induce linear dependence within the system (24). The system determinant collapses to zero causing the matrix solution to fail. Still, this difficulty can be bypassed by adding a pseudo-random perturbation to the Hammersley points' coordinates. Computations have shown that this algorithm works reasonably well.

An alternative that can grant good coverage of uncertainty space (when combined with random point collocation) is the method of least squares. In this approach, a superset of $R+1$ random collocation points is generated where $R > P$. This number of collocation points forces (24) to become an over determined system of equations. The over determined version of system (24) may be written as

$$[\Psi]\vec{\alpha} = \vec{\alpha}^*$$ (25)

where $[\Psi]$ is an $(R+1)\times(P+1)$ matrix of the form

$$[\Psi] = \begin{bmatrix} \Psi_0(\vec{\xi}_0) & \Psi_1(\vec{\xi}_0) & \cdots & \Psi_P(\vec{\xi}_0) \\ \Psi_0(\vec{\xi}_1) & \Psi_1(\vec{\xi}_1) & \cdots & \Psi_P(\vec{\xi}_1) \\ \vdots & \vdots & \ddots & \vdots \\ \Psi_0(\vec{\xi}_{R-1}) & \Psi_1(\vec{\xi}_{R-1}) & \cdots & \Psi_P(\vec{\xi}_{R-1}) \\ \Psi_0(\vec{\xi}_R) & \Psi_1(\vec{\xi}_R) & \cdots & \Psi_P(\vec{\xi}_R) \end{bmatrix}$$ (26)

and $\vec{\alpha}$ is a $(P+1)\times 1$ vector containing the unknown expansion coefficients, , i.e.,

$$\vec{\alpha} = (\alpha_0, \alpha_1, \ldots, \alpha_P)^T$$ (27)

The right hand side of (25) is the $(R+1)\times 1$ vector denoted $\vec{\alpha}^*$ containing the values of the random process evaluated at the $R+1$ collocation points. This vector is written as

$$\vec{\alpha}^* = (\alpha_0^*, \alpha_1^*, \ldots, \alpha_R^*)^T$$ (28)

The classical least squares system of equations is obtained by multiplying (25) by the transpose of polynomial matrix, i.e.,

$$[\Psi]^T[\Psi]\vec{\alpha} = [\Psi]^T\vec{\alpha}^*$$ (29)

The matrix inner product $[\Psi]^T[\Psi]$ is a $(P+1)\times(P+1)$ square matrix. Similarly, $[\Psi]^T\vec{\alpha}^*$ is a vector with $P+1$ elements. With these dimensions, (29) is solvable by standard numerical linear algebra techniques. The specific matrix-vector forms are

$$[\Psi]^T[\Psi] = \begin{bmatrix} \displaystyle\sum_{k=0}^{R}\Psi_{0k}^2 & \displaystyle\sum_{k=0}^{R}\Psi_{0k}\Psi_{1k} & \cdots & \displaystyle\sum_{k=0}^{R}\Psi_{0k}\Psi_{Pk} \\ \displaystyle\sum_{k=0}^{R}\Psi_{1k}\Psi_{0k} & \displaystyle\sum_{k=0}^{R}\Psi_{1k}^2 & \cdots & \displaystyle\sum_{k=0}^{R}\Psi_{1k}\Psi_{Pk} \\ \vdots & \vdots & \ddots & \vdots \\ \displaystyle\sum_{k=0}^{R}\Psi_{Pk}\Psi_{0k} & \displaystyle\sum_{k=0}^{R}\Psi_{1Pk}\Psi_{1k} & \cdots & \displaystyle\sum_{k=0}^{R}\Psi_{Pk}^2 \end{bmatrix} \tag{30}$$

$$[\Psi]^T\vec{\alpha}^* = \begin{bmatrix} \displaystyle\sum_{k=0}^{R}\Psi_{0k}\alpha_k^* \\ \displaystyle\sum_{k=0}^{R}\Psi_{1k}\alpha_k^* \\ \vdots \\ \displaystyle\sum_{k=0}^{R}\Psi_{Pk}\alpha_k^* \end{bmatrix} \tag{31}$$

The classical least squares formulation works well when applied to problems involving the uniform probability distribution. One may recall that uniform probability distribution has a constant weight function $w(\vec{\xi})$ within its probability measure. Other probability distributions have non-constant weight functions. An examination of the above equations reveals that the classical least squares approach does not incorporate the effect of the weight function in a direct manner. The effect of a non-uniform distribution is conveyed only in a tacit manner, by a careful, histographical selection of collocation points. To provide an improved capability for the least squares approach, an alternative formulation does include the effects of weighting the collocation points.

Rigorous least-squares derivations are based upon a minimization of squared error. For the point collocation polynomial chaos problem, the error may be formulated as follows.[24,25] Recall that the polynomial chaos representation for random process α^* is written as

$$\alpha^*(\vec{\xi}) = \sum_{i=0}^{P}\alpha_i\Psi_i(\vec{\xi}) \tag{32}$$

For this analysis, the truncated series is employed. The total squared error E for the chaos expansion may be expressed as a function of the expansion coefficients α_j, $j=0,1,\ldots,P$, i.e.,

$$E(\alpha_0, \alpha_1, \ldots, \alpha_P) = \int_{\Omega(\vec{\xi})} \left(\alpha^*(\vec{\xi}) - \sum_{i=0}^{P} \alpha_i \Psi_i(\vec{\xi}) \right)^2 w(\vec{\xi}) d\vec{\xi} \tag{33}$$

Equation (33) integrates over $\vec{\xi}$ as a continuum. To evaluate the squared error for the collocation points, we apply the Monte Carlo average.[24,25]

$$E(\alpha_0, \alpha_1, \ldots, P) = \frac{1}{R+1} \sum_{j=0}^{R} \left(\alpha^*(\vec{\xi}_j) - \sum_{i=0}^{P} \alpha_i \Psi_i(\vec{\xi}_j) \right)^2 w(\vec{\xi}_j) \tag{34}$$

To minimize the squared error, we set a condition on the first partial derivative.

$$\frac{\partial E}{\partial \alpha_k} = 0, \quad k = 0, 1, \ldots, P \tag{35}$$

By applying (35) to (34), we obtain

$$\frac{\partial E}{\partial \alpha_k} = \frac{1}{Q} \sum_{j=1}^{Q} \frac{\partial}{\partial \alpha_k} \left(\alpha^*(\vec{\xi}_j) - \sum_{i=0}^{P} \alpha_i \Psi_i(\vec{\xi}_j) \right)^2 w(\vec{\xi}_j) = 0, \quad k = 0, 1, \ldots, P \tag{36}$$

After differentiation and substitution, we exchange the order of summation; the result is

$$\sum_{i=0}^{P} \alpha_i \left(\sum_{j=0}^{R} \Psi_i(\vec{\xi}_j) \Psi_k(\vec{\xi}_j) w(\vec{\xi}_j) \right) = \sum_{j=0}^{R} \alpha^*(\vec{\xi}_j) \Psi_k(\vec{\xi}_j) w(\vec{\xi}_j), \quad k = 0, 1, \ldots, P \tag{37}$$

Equation (37) constitutes a system of linear equations. By setting

$$\Phi_{ki} = \sum_{j=0}^{R} \Psi_i(\vec{\xi}_j) \Psi_k(\vec{\xi}_j) w(\vec{\xi}_j) \tag{38}$$

$$G_k = \sum_{j=0}^{R} \alpha^*(\vec{\xi}_j) \Psi_k(\vec{\xi}_j) w(\vec{\xi}_j) \tag{39}$$

the linear system may be written as

$$\sum_{i=0}^{P} \alpha_i \Phi_{ki} = G_k, \quad k = 0, 1, \ldots, P \tag{40}$$

Clearly, the probability weight function is incorporated in both (38) and (39). The system (40) can be solved, like (29), by methods such as LU-decomposition.

3.4 Legendre Polynomial Chaos

For this chaos, the uncertainties are represented by a random vector $\vec{\xi}$ comprised of a set of n random variables, i.e.,

$$\vec{\xi} = (\xi_1, \xi_2, \ldots, \xi_n) \tag{41}$$

In addition to the random character contained in (4), the random process α is also defined in space and time.[14, 15] This process is written as

$$\alpha(\vec{x}, t, \vec{\xi}) = \sum_{j=0}^{P} \alpha_j(\vec{x}, t)\, \Psi_j(\vec{\xi}) \tag{42}$$

Note that this polynomial decomposition, in full form, possesses an infinite number of terms like a typical Fourier series. For practical computations, the series is truncated as in (42) to retain only a finite number of terms. The maximum number of terms, $P+1$, may be computed from the formula

$$P+1 = \frac{(p+n)!}{p!\,n!} \tag{43}$$

where p is the order of the Legendre polynomial set used for the chaos. This total number of expansion terms can be arrived at by combinatorial arguments. Therefore, if p equals five, then Legendre polynomials of orders zero through five are used to form the chaos. The construction of expansion (42) is very important; each term is separated into a deterministic coefficient $\alpha_j(\vec{x}, t)$ and a random tensor product polynomial $\Psi_j(\vec{\xi})$. The tensor product polynomial is a product of single random variable Legendre polynomials. That is to say,

$$\Psi_j(\vec{\xi}) = L_{p1}(\xi_1)L_{p2}(\xi_2)\cdots L_{pn}(\xi_n) \tag{44}$$

Table 2. Legendre Polynomials

Order	Legendre Polynomial
0	$L_0(\xi) = 1$
1	$L_1(\xi) = \xi$
2	$L_2(\xi) = 3\xi^2 - 1$
3	$L_3(\xi) = \xi\,(5\xi^2 - 3)$
4	$L_4(\xi) = 3 - 30\xi^2 + 35\xi^4$
5	$L_5(\xi) = \xi\,(15 - 70\xi^2 + 63\xi^4)$

Legendre polynomial orders $p1, p2, \ldots, pk$ are constrained such that $0 \le pk \le p$, $1 \le k \le n$. An individual Legendre polynomial L_{pk} has algebraic order k. The first six Legendre polynomials are presented in Table 2. Of course, these polynomials are unique up to a constant multiple. With some effort, higher order Legendre polynomials may be calculated by using the Rodrigues formula

$$L_n(\xi) = \frac{1}{2^n \, n!} \frac{d^n(\xi^2 - 1)^n}{d\xi^n} \tag{45}$$

It follows from (44) that Ψ_j has the algebraic order $p1 + p2 + \cdots + pk$. It is computationally advantageous to arrange the terms in (42) by increasing algebraic order beginning with the zeroth order term, then the first order terms and so forth. For two random variables ξ_1 and ξ_2, this ordering of the Ψ_j can be determined from organization shown in Table 3. Those Ψ_j possessing

Table 3. Organization of Legendre Polynomials for Two Random Variables

$\Psi_0 = L_0(\xi)L_0(\xi)$	$\Psi_2 = L_0(\xi)L_1(\xi)$	$\Psi_5 = L_0(\xi)L_2(\xi)$	$\cdots$	$\Psi = L_0(\xi)L_p(\xi)$
$\Psi_1 = L_1(\xi)L_0(\xi)$	$\Psi_4 = L_1(\xi)L_1(\xi)$	$\Psi_8 = L_1(\xi)L_2(\xi)$	$\cdots$	$\Psi = L_1(\xi)L_p(\xi)$
$\Psi_3 = L_2(\xi)L_0(\xi)$	$\Psi_7 = L_2(\xi)L_1(\xi)$	$\Psi = L_2(\xi)L_2(\xi)$	$\cdots$	$\Psi = L_2(\xi)L_p(\xi)$
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
$\Psi = L_p(\xi)L_0(\xi)$	$\Psi = L_p(\xi)L_1(\xi)$	$\Psi = L_p(\xi)L_2(\xi)$	$\cdots$	$\Psi_{p^2-1} = L_p(\xi)L_p(\xi)$

the same algebraic order are located on diagonals (lower left to upper right) in this table. The first diagonal has order zero; the second diagonal (Ψ_1 and Ψ_2) has order one; the third diagonal (Ψ_3, Ψ_4 and Ψ_5) has order two, and the pth diagonal has order p-1. The remaining diagonals follow suit, culminating with the bottom right corner table entry with order $p^2 - 1$. The numbering of the Ψ_j follows that shown in the Table 3, but the larger j indices are omitted because of the lengths of the expressions. Still, individual indices are not difficult to discern because the length of each diagonal is known. That is, the number of terms possessing the same algebraic order is the same as the number of elements in the associated diagonal.

To support accurate calculations of statistical properties via equations (17), (22) and (23), it is necessary to normalize the Legendre polynomials. The normalized magnitude "norm" for an orthogonal polynomial $f(\xi)$ may be calculated as follows. The squared norm of $f(\xi)$, denoted $\langle f^2 \rangle$, is given by

$$\langle f^2 \rangle = \int_{\Omega(\xi)} f^2(\xi) \, dw(\xi) \tag{46}$$

In equation (46), $\Omega(\xi)$ is the domain of the random variable ξ while $dw(\xi)$ is the probability measure associated with the random variable. The Legendre chaos is associated with a standard uniform random variable ξ where $\xi \in [-1, 1]$. The mean of this random variable is zero, and the probability measure is given by

$$dw(\xi) = \frac{d\xi}{2} \qquad (47)$$

With the use of (47), the squared norms for the Legendre polynomials found in Table 2 are computed and recorded in Table 4.

Table 4. Squared Norms for the Legendre Polynomials in One Random Variable

Order	Squared Norm
0	1
1	1/3
2	4/5
3	4/7
4	64/9
5	64/11

3.5 Hermite Polynomial Chaos

A distinct advantage of the polynomial chaos method is the generality of its mathematical form. The equation for the expansion, the structure of the uncertainty vector and number of terms in the expansion remain unchanged. Only the orthogonal polynomial set and the probability weight function (measure) change. The Hermite chaos is based upon the standard normal (Gaussian) distribution, i.e.,

$$w(\vec{\xi}) = \frac{1}{(2\pi)^{n/2}} \exp(\tfrac{1}{2} \vec{\xi} \bullet \vec{\xi}) \qquad (48)$$

Equation (48) is suited for an uncertainty vector of arbitrary integer length n. For a chaos involving only one random variable ξ (the uncertainty),

$$w(\xi) = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{\xi^2}{2}\right) \qquad (49)$$

Similarly, for two random variables $\vec{\xi} = (\xi_1, \xi_2)$, the weight function is

$$w(\vec{\xi}) = \frac{1}{2\pi}\exp\left(\frac{\xi_1^2 + \xi_1^2}{2}\right) \tag{50}$$

The Hermite polynomials constitute the orthogonal spanning set required for this chaos. The Hermite polynomials for one random variable may be calculated from the Rodrigues formula

$$H_j(\xi) = \exp\left(\frac{1}{2}\xi^2\right)(-1)^j \frac{\partial^j}{\partial \xi^j}\left[\exp\left(-\frac{1}{2}\xi^2\right)\right] \tag{51}$$

The first five of these polynomials are listed in Table 5 along with their squared norms.

Table 5. Hermite Polynomials

Order	Hermite Polynomial	Norm
0	$H_0(\xi) = 1$	1
1	$H_1(\xi) = \xi$	1
2	$H_2(\xi) = \xi^2 - 1$	2
3	$H_3(\xi) = \xi^3 - 3\xi$	6
4	$H_4(\xi) = 3 - 6\xi^2 + \xi^4$	24

For systems involving more than one Gaussian random variable, this chaos is still applicable, but the calculation of Hermite polynomials is more difficult. These computations are reserved for a future report. The chaos formulations presented in this section and the previous one are well suited for the example problems that follow.

4.0 RESULTS AND DISCUSSION

In this section, four test problems are described for the polynomial chaos solution. The first three problems are designed for solution by the Legendre chaos. The final problem applies the Hermite chaos to resolve the uncertainty associated with shocked gas dynamics configuration. The exact statistical parameters for the first four cases are derived in the appendices.

4.1 Test Problem 1

This test case, designed by the author, involves a random process operating on one random variable $\xi \in [-1,1]$. The random process $f(\xi)$ is

$$f(\xi) = 1 - \frac{1}{3}\left(\xi^2 + \xi^4 + \xi^6\right) \tag{52}$$

Statistical parameters for this random process are computed through the use of a fifth order Legendre polynomial chaos. The exact solution for this problem is provided in Appendix A. In the terminology of Section 2, $p = 5$, and $n = 1$, so

$$P + 1 = \frac{(5+1)!}{5!1!} = 6 \tag{53}$$

For a direct polynomial chaos solution, a system of 6 equations in 6 unknowns must be solved. The equations are formulated at the 6 collocation points shown in Table 6. The mean and standard deviation calculated for this test problem are shown in Table 7 and compared with the exact calculations. The agreement between the chaos estimates and the exact parameters is quite good especially given the low number of collocation points.

Table 6. Collocation Point Coordinates for Test Problem 1

Point No.	ξ
1	-0.90
2	-0.60
3	-0.30
4	0.20
5	0.55
6	0.95

Table 7. Statistical Parameters for Test Problem 1

Parameter	5th Order Chaos	Exact
Mean	0.77238	0.7746
Standard Deviation	0.26228	0.26258

4.2 Test Problem 2

This test problem, again developed by the author, is cast in terms of a random process f operating on one random variable $\xi \in [-1,1]$. Specifically,

$$f(\xi) = \frac{1}{4}\left(1 - \xi^2\right)\left(\sin(10\xi) + 3\right) \tag{54}$$

The fifth order Legendre chaos is also applied in estimating the mean and standard deviation for this random process. As shown for the previous case, six collocation points are required for this test problem. The same list of collocation points provided in Table 6 is used for this problem. The Legendre chaos is solved for this test case, and the estimated statistical parameters are listed and compared against the exact parameters in Table 8.

Table 8. Collocation Point Coordinates for Test Problem 2

Parameter	5th Order Chaos	Exact
Mean	0.49401	0.50
Standard Deviation	0.34134	0.26048

For the low number of collocation points applied here, the agreement between the estimated and exact parameters is reasonably good.

4.3 Test Problem 3

The first two test problems addressed by this report involve one random variable and serve to verify the polynomial chaos solution algorithms discussed in Section 2. This test problem is cast in two random variables and has a mixture of algebraic and transcendental functions.[15] Specifically,

$$f(x_1, x_2) = \ln(1 + x_1^2)\sin(5x_2) \tag{55}$$

where x_1 and x_2 are uniform random variables with mean 2.0 and a coefficient of variation (CoV) of 20%. The mean and CoV can be used to identify the domain of x_1 and x_2, i.e.,

$$x_1, x_2 \in [a,b] = [2.0 - 0.4\sqrt{3}, 2.0 + 0.4\sqrt{3}] \tag{56}$$

Random variables x_1 and x_2 are regarded as functions of standard uniform random variables $\xi_{1,2}$ with mean zero and standard deviation $\sqrt{3}^{-1}$. That is, $\xi \in [-1,1]$. The domain of $\xi_{1,2}$ can be mapped onto the domain of $x_{1,2}$ (and vice versa) by the transformation

$$x_j = a + \left(\frac{\xi_j + 1}{2}\right)(b - a) \tag{57}$$

18

The exact statistical parameters for this random process are described in Appendix C. The number of terms required for the Legendre polynomial chaos is calculated as

$$P + 1 = \frac{(5+2)!}{5!2!} = 21 \tag{58}$$

This polynomial chaos is solved for two different point distribution schemes. The first method of distributing collocation points is the random method. A linear congruential random number generator is used to distribute points in the interval [0,1].[26] Then these points are mapped onto the domain of ξ for use in the random process formulas (55) and (57). A direct solution is performed for 21 collocation points. These points are listed in Table 9. Secondly, a least squares solution is accomplished for 100 collocation points. For brevity, these points are not listed here. The fifth order direct and least squares solutions for this problem are listed and compared with exact values in Table 10.

Table 9. Random Collocation Points for the Direct Solution of Problem 3

Point	ξ_1	ξ_2	Point	ξ_1	ξ_2
1	0.9999974	0.9555932	12	0.4861153	0.1398800
2	0.6545904	-0.2987570	13	0.9636399	-0.1042775
3	0.7917758	-0.6235767	14	-0.5915973	-0.9762128
4	-0.4539059	-0.7957101	15	0.7914310	-0.4188466
5	0.5000229	-0.1146452	16	0.4447752	-0.6623921
6	-0.8423904	-0.0558344	17	-0.8242336	-0.8933002
7	-0.4100209	0.7791101	18	0.3031493	-0.9700800
8	0.5027170	-0.8346537	19	-0.1349102	0.5640060
9	-0.0248729	-0.0391431	20	-0.7509418	0.9213717
10	0.1213641	-0.2343712	21	-0.5064132	0.7136617
11	0.9234417	0.2839582			

Table 10. Statistical Parameters for Test Problem 3 with Random Point Distributions

Parameter	Direct	Least Squares	Exact
Mean	0.0729048	0.078819	0.079169
Standard Deviation	1.14888	1.11923	1.12413

A second method of solving this problem involves the use of Hammersley sampling points. Both the direct and least squares algorithms are applied in estimate the statistical parameters for this case. For a direct linear solution, the 21 Hammersley collocation points are listed in Table 11. Although not listed here, 100 Hammersley points are used for a least squares solution. Estimates of the mean and standard deviation for problem 3 based upon the Hammersley point distributions are compared against the exact values in Table 12.

It is interesting to note that, on the whole, polynomial chaos estimates are reasonably accurate for this problem, but the accuracy of the least squares estimates for random point distributions compare more favorably to the exact values. It is a little shocking to see that estimates based upon the Hammersley distributions perform more poorly, even though the Hammersley distribution provides better coverage of the sample space. The least squares analysis improves the estimates made by using both random and Hammersley point distributions.

Table 11. Hammersley Collocation Points for the Direct Solution of Problem 3

Point	ξ_1	ξ_2	Point	ξ_1	ξ_2
1	0.9999974	0.9555932	12	0.4861153	0.1398800
2	0.6545904	-0.2987570	13	0.9636399	-0.1042775
3	0.7917758	-0.6235767	14	-0.5915973	-0.9762128
4	-0.4539059	-0.7957101	15	0.7914310	-0.4188466
5	0.5000229	-0.1146452	16	0.4447752	-0.6623921
6	-0.8423904	-0.5583447	17	-0.8242336	-0.8933002
7	-0.4100209	0.7791101	18	0.3031493	-0.9700800
8	0.5027170	-0.8346537	19	-0.9700800	0.5640060
9	-0.0248729	-0.0391431	20	-0.7509418	0.9213717
10	0.1213641	-0.2343712	21	-0.5064132	0.7136617
11	0.9234417	0.2839582			

Table 12. Statistical Parameters for Test Problem 3 with Hammersley Point Distributions

Parameter	Direct	Least Squares	Exact
Mean	0.061475	0.069076	0.079169
Standard Deviation	1.183351	1.123245	1.12413

4.4 Test Problem 4

This test case is the last of the truly "academic" demonstration problems addressed here. The random process to be considered operates on four independent uniform random variables. The random process is defined as

$$f(x_1, x_2, x_3, x_4) = \exp[1.5(x_1 + x_2 + x_3 + x_4)] \tag{59}$$

where random variables $x_i = x_i(\xi_i)$, $i = 1, \ldots, 4$ are functions of the standard uniform random variables ξ_i, where $\xi_i \in [-1,1]$.[15] Random variables x_i have a mean value of 0.4 and a coefficient of variation (CoV) of 0.4. With the use of this information, it can be shown that the domain for x_i is

$$[a,b] = [0.4 - 0.08\sqrt{12}, 0.4 + 0.08\sqrt{12}] \tag{60}$$

For a fifth order polynomial chaos solution, the number of terms for the expansion is calculated as follows.

$$P + 1 = \frac{(5+4)!}{5!4!} = 126 \tag{4-10}$$

A term in the expansion polynomial, following equation (44), has the form

$$\Psi_n = L_{n1}(\xi_1)\, L_{n2}(\xi_2)\, L_{n3}(\xi_3)\, L_{n4}(\xi_4) \tag{4-10a}$$

where $0 \le nj \le 5$, $j = 1, \ldots, 4$. In this case, a large number of terms is required to determine the statistical parameters with fifth order accuracy. This outcome is referred to as the "curse of dimensionality".[27] That is, for a given level of accuracy, the number of expansion terms increases significantly for each additional random variable. As with the previous test cases, the fifth order Legendre chaos is applied to estimate the mean and standard deviation for equation (59). The collocation points are too numerous to list here. Both the direct solution (126 collocation points) and the least squares solution (200 collocation points) have been computed for this problem. The results are presented in Table 13. Because of the poorer performance of the Hammersley point set used in the previous test case, it is not used here. For the random point sets, the results are quite good with the least squares case granting only minor improvements over the direct method. The results for these four test problems indicate that the Legendre chaos performs well by rendering sound estimates for statistical parameters.

Table 13. Statistical Parameters for Test Problem 4 with Random Point Distributions

Parameter	Direct	Least Squares	Exact
Mean	12.3519	12.3602	12.3609
Standard Deviation	6.1631	6.1569	6.1556

4.5 Test Problem 5

The preceding problems test the basic operation of the polynomial chaos algorithms given known, deterministic function forms. The uncertainty in the system is provided by the random variable(s) providing input data. This test case is an actual application of this idea. Here, the input uncertainty is provided by changing a physical boundary condition for a computational fluid dynamics (CFD) solution.[14, 15, 21] The algebraic functions used in the previous test cases are replaced by separate CFD solutions for each "randomly" chosen boundary condition. The Hermite chaos is applied to solve the classical oblique shock wave problem. A Mach 3 flow field of a calorically perfect gas encounters a wedge. To satisfy this solid surface inviscid boundary condition, the flow must turn at the cusp of the wedge or ramp. Physics dictates that the turning occurs through an oblique shock wave originating the wedge's cusp. This scenario is illustrated in Figure 1. The uncertainty is provided by perturbations in the wedge angle. The mean wedge angle $\bar{\theta}$ is five degrees, and the distribution of possible wedge angles is Gaussian with a coefficient of variation of 10%.[21] Based upon this information, the standard deviation for the wedge angle distribution is
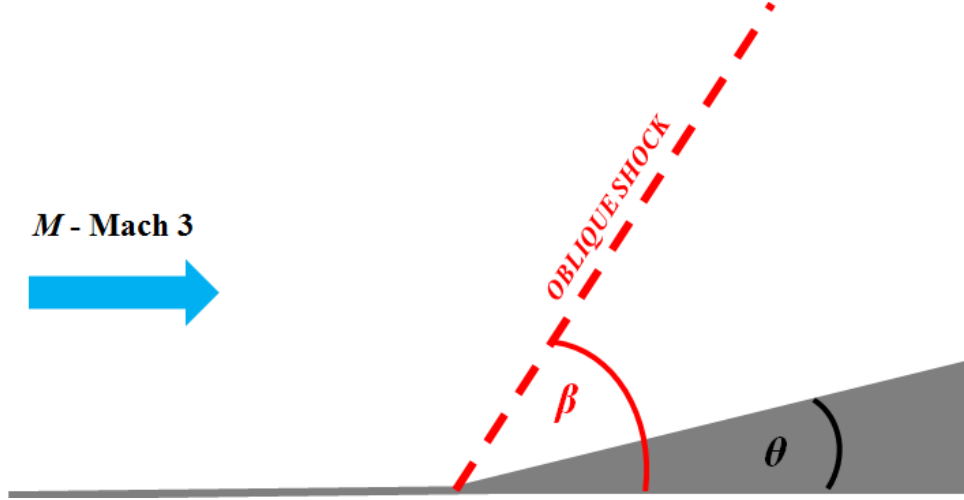
Figure 1. Oblique Shock Wave Problem Geometry

$$\sigma = 0.10 \quad \bar{\theta} = 0.5° \tag{63}$$

The probability distribution for the wedge angle is given by

$$w(\theta) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(\theta - \bar{\theta})^2}{2\sigma^2} \right] \tag{64}$$

Hence,

$$\frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left[-\frac{(\theta - \bar{\theta})^2}{2\sigma^2} \right] d\theta = 1 \tag{65}$$

By using the transformation

$$\xi = \frac{\theta - \bar{\theta}}{\sigma} \tag{66}$$

we obtain the standard normal distribution

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{\xi^2}{2} \right) d\xi = 1 \quad \Rightarrow \quad w(\xi) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\xi^2}{2} \right) \tag{67}$$

Equation (66) can be rewritten as follows.

$$\theta = \bar{\theta} + \xi\sigma \tag{68}$$

22

By comparing (64) and (67), we note that the standard deviation for the standard normal distribution is unity, so to properly sample wedge angles for this problem, samples ξ_j must be chosen so that $-2 \leq \xi_j \leq 2$. A fourth order Hermite chaos may be used to estimate statistical properties for pressure throughout the flow field. Since only one random input variable (wedge angle) is involved, the total number of expansion terms is computed as follows.[21]

$$P + 1 = \frac{(4+1)!}{4!\,1!} = 5 \tag{69}$$

With the use of these equations, the sampled wedge angles are listed in Table 13.

Table 14. Sampled Wedge Angles for the Oblique Shock Wave Case

j	ξ_j	θ_j
1	-2	4.0
2	-1	4.5
3	0	5.0
4	1	5.5
5	2	6.0

To statistically sense how the flow field is perturbed by the boundary fluctuation, the flow field is sampled at the three points listed in Table 14. Points 1 and 3 differ for each wedge angle since point 1 is situated in the shock wave while point 3 is on the wedge surface. As a result, the y coordinate of this point differs for each wedge angle. In Reference 15, a fixed set of sampling points, a total of three, is used for all wedge angles. This approach is not applied here since an undisclosed interpolation algorithm is applied in Reference 15 to refocus the data at the sample point locations. Since the points in Table 14 are relatively close to the points used in the archival reference, we assume that their values are representative of the random process at the fixed points.

Table 15. Sample Point Locations

Wedge Angle (º)	4.0	4.5	5.0	5.5	6.0
Point	x	y	y	y	y	y
1	0.8984	0.3669	0.3675	0.3822	0.3879	0.3969
2	0.8984	0.2321	0.2333	0.2312	0.2327	0.2311
3	0.8984	0.0644	0.0722	0.0813	0.0879	0.0985

The CFD solution for each wedge angle is computed by using the Large Eddy Simulation with LInear Eddy modeling in 3 Dimensions (LESLIE3D) multiphase physics computer program. LESLIE3D is developed by Professor Suresh Menon at the Georgia Institute of Technology. It is a multi-block, massively parallel computer program with extensive physics capabilities. Structured grids are developed for each wedge angle, and numerical solutions are computed for freestream Mach number 3.0, sea level atmospheric pressure and temperature 300ºK. A plot of the velocity field for the 5º wedge is shown in Figure 2. LESLIE3D resolves the
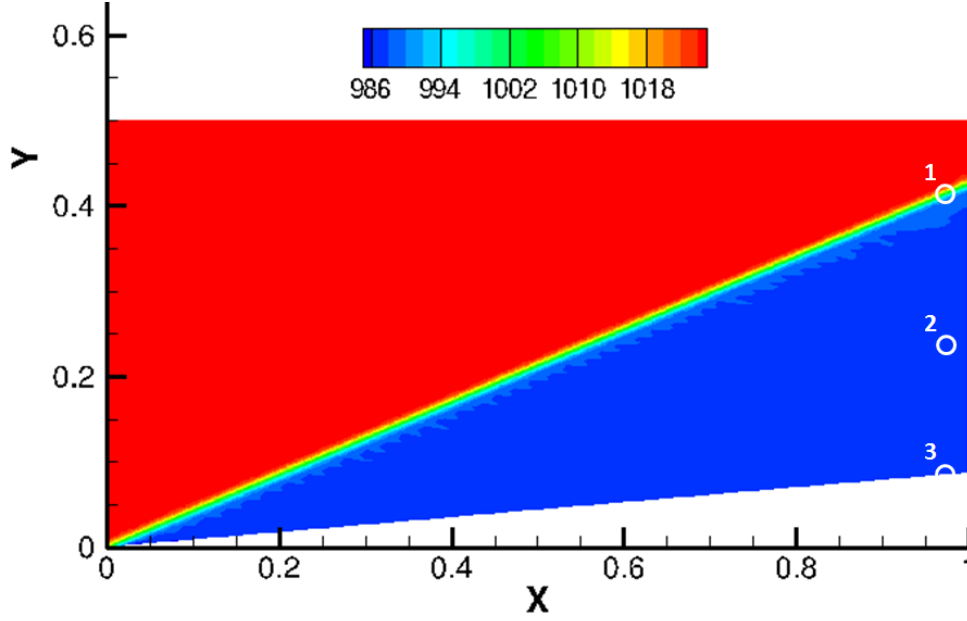
Figure 2. Oblique Shock Solution X-Velocity Plot for the 5º Wedge

shock wave accurately confirming the shock angle mandated by the $\theta - \beta - M$ relationship.[27] For the 5º wedge, the Cartesian x-velocity field is show in Figure 2. The pressure field is recorded at the sample points (listed in Table 14 and shown in Figure 2) then post-processed by using the Hermite polynomial chaos. The ratio of pressure versus freestream pressure is the random process considered by the chaos. The computed mean and standard deviation are shown in Tables 15 and 16, respectively, for this problem and compared with archived results taken from Reference 15.

Table 16. Means Computed for P/P_{ref} via 4th Order Hermite Chaos

Sample Point	Mean	Archived
1	1.2091	1.11433
2	1.4868	1.45484
3	1.4651	1.45472

Table 17. Standard Deviations Computed for P/P_{ref} via 4th Order Hermite Chaos

Sample Point	Standard Deviation	Archived
1	0.07435	0.14033
2	0.07036	0.05242
3	0.09073	0.05227

Overall, the agreement between the present Hermite chaos estimates and the archived estimates is good but compares less favorably than the other test problems. There are a number of reasons for this less than inspirational comparison. Our method utilizes a different CFD computer program and grid than does the archival reference. Also, the LESLIE3D solution is performed

for an Oxygen-Nitrogen mixture with air mass fractions and a ratio of specific heats of 1.35. Also, the archival solution employs interpolation to fixed sample points. This interpolation scheme is not documented, so it cannot be replicated for the present calculations. For future problems, the author will devise, implement and document an interpolation procedure to bridge the gap between different stochastic realizations of a more complicated problem of choice.

5.0 CONCLUSIONS

This expository report has described basic aspects of the polynomial chaos method for representing stochastic or random processes. These methods evolve from the homogeneous chaos introduced by Wiener.[10] In summary, random processes can be represented by finite series of orthogonal polynomials. The bulk of this work concentrates on the point collocation non-intrusive polynomial chaos method due to researchers such as Walters and Hosder.[15] Non-intrusive methods permit statistical estimates without altering the governing equations. Instead, polynomial expansions are developed at a set of collocation points selected for a set of input random variables. These random variables, representing the system uncertainties, drive the random aspects of the overall random or stochastic process. Although the point collocation method renders non-unique results, its estimates have shown to be sufficiently accurate for the included test problems. In each case, the present calculations agree well with archived (or exact) estimates.

Polynomial chaos methods are not without difficulties. Perhaps the most prominent difficulty is that of dimensionality. The combination of polynomial order and the number of random variables (uncertainties) requires an increasing number of expansion terms. To resolve the coefficients for a system of n terms, an $n \times n$ matrix must be solved. Matrix solutions do require significant computer resources and time. Moreover, for a time and space dependent system, the chaos must be solved at each space location and time of interest. It is in this sense that the polynomial chaos method begins to approach the workload involved in a Monte Carlo simulation. In addition, the point collocation, non-intrusive polynomial chaos method produces results that are not unique. Rather, the results depend, somewhat, on the choice of collocation points. The analyst must ensure that the random space receives sufficient coverage. Moreover, it must possess the appropriate level of randomness with the appropriate distribution for the uncertainties. Other analyses have shown that these methods have difficulties in addressing higher magnitude uncertainties, and there are questions concerning the accuracy of polynomial expansions.[28] In other instances, the convergence of polynomial chaos expansions may be slow, and a given expansion's accuracy may not increase with the inclusion of more terms. Statistical moments of third or higher order may not be accurate.[29]

In a future report, these investigations will continue. The non-intrusive polynomial chaos method will be applied to a series of gas dynamics problems involving strongly shocked flow fields. The problems, their geometries and associated physics will have greater complexity that any of the test cases shown in the present work. A number of uncertainties will be examined, particularly those involving the boundary.

REFERENCES

1. Najm, H.N., "Uncertainty quantification and polynomial chaos techniques in computational fluid dynamics", *Annual Review of Fluid Mechanics*, Vol. 41, 2009, pp. 35-52.

2. Ross, S.M., *Introduction to Probability Models*, 4th Ed., Academic Press, Boston, Massachusetts, 1989.

3. Cameron, R.H. and Martin, W.T., "The orthogonal development of non-linear functionals in series of Fourier-Hermite functionals", *Annals of Mathematics*, Vol. 48, No. 2, pp. 385-392.

4. Ghanem, R.G. and Spanos, P.D., *Stochastic Finite Elements, A Spectral Approach*, Rev. Ed., Dover Publications, Mineola, New York, 2003.

5. Pettersson, M.P., *Uncertainty Quantification and Numerical Methods for Conservation Laws*, Doctoral Dissertation, Institute for Computational and Mathematical Engineering, Stanford University, 2012.

6. Hammersley, J.M. and Handscomb, D.C., *Monte Carlo Methods*, Methuen's Monographs on Applied Probability and Statistics, Bartlett, M.S., Ed., Fletcher & Son, Ltd., Norwich, Great Britain, 1964.

7. Anderson, J.B. and Long, L.N., "Direct Monte Carlo simulation of chemical reaction systems: prediction of ultrafast detonations", *Journal of Chemical Physics*, Vol. 118, No. 7, 2003, pp. 3102-3110.

8. Johansen, A.M. and Evers, L., *Monte Carlo Methods*, Lecture Notes, University of Bristol, Department of Mathematics, Bristol, England, 2007.

9. Oden, J.T. and Demkowicz, L., *Applied Functional Analysis*, 2nd Ed., Computational Mechanics and Applied Mathematics, CRC Press, Boca Raton, Florida, 1996.

10. Weiner, N., "The homogeneous chaos", *American Journal of Mathematics*, Vol. 60, No. 4, 1938, pp. 897-936.

11. Xiu, D. and Karniadakis, G.E., "The Weiner-Askey polynomial chaos for stochastic differential equations", *SIAM Journal of Scientific Computing*, Vol. 24, No. 2, 2002, pp. 619-644.

12. Sandu, A., Sandu, C. and Ahmadian, M., "Modeling multibody systems with uncertainties. Part I: Theoretical and computational aspects", *Multibody System Dynamics*, Vol. 15, 2006, pp. 373-395.

13. Soize, C. and Ghanem, R., "Physical systems with random uncertainties: chaos representations with arbitrary probability measure", *SIAM Journal of Scientific Computing*, Vol. 26, No. 2, 2004, pp. 395-410.

14. Hosder, S. and Walters, R.W., "Non-Intrusive Polynomial Chaos Methods for Uncertainty Quantification in Fluid Dynamics", AIAA 2007-129, 48th AIAA Aerospace Sciences Meeting, 4-7 January 2010, Orlando, Florida.

15. Hosder, S., Walters, R.W. and Balch, M., "Efficient Sampling for Non-Intrusive Polynomial Chaos Applications with Multiple Uncertain Input Variables", AIAA 2007-1939, 48th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference, 23-26 April 2007, Honolulu, Hawaii.

16. Abramowitz, M. and Stegun, I.A., Eds., *Handbook of Mathematical Tables with Formulas, Graphs and Mathematical Tables*, Dover Publications, Mineola, New York, 1965.

17. Knio, O.M. and Le Maitre, O.P., "Uncertainty propagation in CFD using polynomial chaos decomposition", *Fluid Dynamics Research*, Vol. 38, No. 9, 2006, pp. 616-640.

18. Eldred, M.S. and Burkardt, J., "Comparison of Non-Intrusive Polynomial Chaos and Stochastic Collocation Methods for Uncertainty Quantification", AIAA 2009-976, 47th Aerospace Sciences Meeting, 5-8 January 2009, Orlando, Florida.

19. Burden, R.L., Faires, J.D. and Reynolds, A.C., *Numerical Analysis*, 2nd Ed., Prindle, Weber & Schmidt, Boston, Massachusetts, 1981.

20. Walters, R.W., "Towards Stochastic Fluid Mechanics Via Polynomial Chaos", AIAA 2003-0413, 41st Aerospace Sciences Meeting, 6-9 January 2003, Reno, Nevada.

21. Hosder, S., Walters, R.W. and Perez, R., "A Non-Intrusive Polynomial Chaos Method for Uncertainty Propagation in CFD Simulations", AIAA 2006-891, 44th AIAA Aerospace Sciences Meeting, 9-12 January 2006, Reno, Nevada.

22. Giunta, A.A., Wojkiewicz, Jr., S.F. and Eldred, M.S., "Overview of Modern Design of Experiments Methods for Computational Simulations", AIAA 2003-649, 41st Aerospace Sciences Meeting, 6-9 January 2003, Reno, Nevada.

23. Wong, T.-T., Luk, W.-S. and Heng, P.-A., "Sampling with Hammersley and Halton Points", *Journal of Graphics Tools*, Vol. 2, No. 2, 1997, pp. 9-24.

24. Cheng, H. and Sandu, A., "Collocation Least-Squares Polynomial Chaos Method", High Performance Computing Symposium, April 2010, Orlando, Florida.

25. Cheng, H., *Uncertainty Quantification and Uncertainty Reduction Techniques for Large Scale Simulations*, Doctoral Dissertation, Virginia Polytechnic Institute and State University, July 15, 2009, Blacksburg, Virginia.

26. L'Ecuyer, P., "Uniform random number generation", *Annals of Operations Research*, Vol. 53, 1994, pp. 77-120.

27. Anderson, J.D., *Modern Compressible Flow: With Historical Perspective*, 2nd Ed., McGraw-Hill, New York, New York, 1990.

28. Debusschere, B.J., Najm, H.N., Pébay, P.P., Knio, O.M., Ghanem, R.G. and Le Maître, O.P., "Numerical challenges in the use of polynomial chaos representations for stochastic processes", *SIAM Journal of Statistical Computing*, Vol. 26, No. 2, 2004, pp. 698-719.

29. Field, R.V., Jr. and Grigoriu, M., "On the accuracy of the polynomial chaos approximation", *Probabilistic Engineering Mechanics*, Vol. 19, 2004, pp. 65-80.

Distribution A

APPENDIX A

DIRECT STATISTICAL ANALYSIS FOR TEST PROBLEM 1

This problem is designed to be a simple test case for the Legendre non-intrusive polynomial chaos. Possessing a constant integration measure, the calculation of statistical parameters is greatly simplified requiring only the evaluation of basic integral averages. This test case involves a random process f operating on a single random variable $\xi \in [-1,1]$. This random process is written as

$$f(\xi) = 1 - \frac{1}{3}\left(\xi^2 + \xi^4 + \xi^6\right) \tag{A-1}$$

For this random process, the probability measure is

$$w(\xi)d\xi = \frac{1}{2}d\xi \tag{A-2}$$

The average, or expected value, for f is computed as follows.

$$E(f) = \frac{1}{2}\int_{-1}^{1}\left[1 - \frac{1}{3}\left(\xi^2 + \xi^4 + \xi^6\right)\right]d\xi \tag{A-3}$$

By evaluating integrals, we obtain

$$E(f) = \frac{1}{2}\left[\xi - \frac{1}{3}\left(\frac{\xi^3}{3} + \frac{\xi^5}{5} + \frac{\xi^7}{7}\right)\right]\Big|_{-1}^{1} \tag{A-4}$$

The mean for this random process is therefore

$$E(f) = \frac{244}{315} \approx 0.7746. \tag{A-5}$$

For this problem, the computation of the variance is similar. Recall that the definition of the variance is

$$\text{var}(f) = \sigma^2 = E(f^2) - (E(f))^2 \tag{A-6}$$

The first term in (A-6)

$$E(f^2) = \frac{1}{2}\int_{-1}^{1}\left[\frac{1}{3}(1-\xi^2) + \frac{1}{3}(1-\xi^4) + \frac{1}{3}(1-\xi^4)\right]^2 d\xi \tag{A-7}$$

Algebra can be employed to simplify the integrand obtaining

$$E(f^2) = \frac{1}{2}\int_{-1}^{1}\left[1 - \frac{1}{9}\left(6\xi^2 + 5\xi^4 + 4\xi^6 - 3\xi^8 - 2\xi^{10} - \xi^{12}\right)\right]d\xi \tag{A-8}$$

This integral may be evaluated as follows.

$$E(f^2) = \frac{1}{2}(2) - \frac{1}{18}\left[6\frac{\xi^3}{3} + 5\frac{\xi^5}{5} + 4\frac{\xi^7}{7} - 3\frac{\xi^9}{9} - 2\frac{\xi^{11}}{11} - \frac{\xi^{13}}{13}\right]_{-1}^{1} \tag{A-9}$$

By simplifying, this moment is

$$E(f^2) = 1 - \frac{1}{9}\left(3 + \frac{4}{7} - \frac{1}{3} - \frac{2}{11} - \frac{1}{13}\right) \approx 0.66896 \tag{A-10}$$

Substitution of (A-7) and (A-5) into (A-6), the variance can be computed as

$$\mathrm{var}(f) = \sigma^2 = 0.66896 - (0.7746)^2 = 0.068949 \tag{A-11}$$

Accordingly, the standard deviation is

$$\sigma = 0.26258 \tag{A-12}$$

Distribution A

APPENDIX B

DIRECT STATISTICAL ANALYSIS FOR TEST PROBLEM 2

This problem is also a simple test case for the Legendre chaos, but it is designed to incorporate a transcendental function into the random process. Again, the random process operates on a single random variable $\xi \in [-1,1]$, and it is defined as

$$f(\xi) = \frac{1}{4}(1 - \xi^2)[\sin(10\xi) + 3] \tag{B-1}$$

The mean of this random process may be computed as follows.

$$E(f) = \int_{-1}^{1} \frac{1}{4}(1 - \xi^2)[\sin(10\xi) + 3]\frac{1}{2}d\xi \tag{B-2}$$

$$E(f) = \frac{1}{8}\int_{-1}^{1} (1 - \xi^2)[\sin(10\xi) + 3]d\xi \tag{B-3}$$

As one can see, the probability measure remains the same as in the previous case. Equation (B-3) is evaluated as shown below.

$$E(f) = \frac{1}{8}\left[\int_{-1}^{1}\sin(10\xi)d\xi + 3\int_{-1}^{1}d\xi - \int_{-1}^{1}\xi^2\sin(10\xi)d\xi - 3\int_{-1}^{1}\xi^2d\xi \right] \tag{B-4}$$

The third integral in (B-4) can be evaluated by performing a detailed integration by parts as

$$\int_{-1}^{1}\xi^2\sin(10\xi)d\xi = 0 \tag{B-5}$$

Intuitively, this integral may be easily computed by realizing that the integrand is anti-symmetric, the product of odd and even functions. For this reason, it must equal zero. Hence,

$$E(f) = \frac{1}{8}\left[\int_{-1}^{1}\sin(10\xi)d\xi + 3\int_{-1}^{1}d\xi - 3\int_{-1}^{1}\xi^2d\xi \right] \tag{B-6}$$

By integrating, we have that

$$E(f) = \frac{1}{8}\left[-\frac{\cos(10\xi)}{10} + 3\xi - \xi^3 \Big|_{-1}^{1} \right] \tag{B-7}$$

$$E(f) = \frac{1}{8}\left[-\frac{\cos(10)}{10} + 2 + \frac{\cos(10)}{10} + 2\right] = \frac{1}{2} \qquad \text{(B-8)}$$

By using similar means, the variance can be calculated. First, the second moment of f is determined, i.e.,

$$E(f^2) = \int_{-1}^{1} \frac{1}{16}\left(1 - 2\xi^2 + \xi^4\right)\left(\sin^2(10\xi) + 6\sin(10\xi) + 9\right)\frac{1}{2}d\xi \qquad \text{(B-8)}$$

By expanding the integrand, we have that

$$E(f^2) = \frac{1}{32}\int_{-1}^{1}\left[\sin^2(10\xi) + 6\sin(10\xi) + 9 - 2\xi^2\sin^2(10\xi) - 12\xi^2\sin(10\xi)\right. \qquad \text{(B-9)}$$
$$\left. - 18\xi^2 + \xi^4\sin^2(10\xi) + 6\xi^4\sin(10\xi) + 9\xi^4\right]d\xi$$

With a significant amount of effort, the integrals in (B-9) can be evaluated by using multiple stages of integration by parts and the half-angle formulas. The result is

$$E(f^2) = \frac{1}{32}\left[\frac{152}{15} + \frac{1657}{40000}\sin(20) + \frac{3}{20000}\cos(20)\right] = 0.31785 \qquad \text{(B-10)}$$

Recalling the variance formula

$$\text{var}(f) = E(f^2) - (E(f))^2 \qquad \text{(B-11)}$$

The variance is computed, through (2-8), (2-10) and (2-11) as

$$\text{var}(f) = \sigma^2 = 0.31785 - (1/2)^2 = 0.0678 \qquad \text{(B-12)}$$

As a result, the standard deviation becomes

$$\sigma = 0.26048 \qquad \text{(B-13)}$$

APPENDIX C

DIRECT STATISTICAL ANALYSIS FOR TEST PROBLEM 3

This problem provides a two-dimensional validation test case for the Non-Intrusive Polynomial Chaos method presented earlier in this report. It involves a non-linear function g of two random variables, i.e.,

$$g(x_1, x_2) = \ln(1 + x_1^2)\sin(5x_2) \tag{C-1}$$

where x_1 and x_2 are uniform random variables with common mean 2.0 and a common coefficient of variation (CoV) of 20%.[C-1] For convenient reference, the CoV is defined as the ratio of the standard deviation to the mean. i.e.,

$$CoV = \frac{\sigma}{\mu} \tag{C-2}$$

These uniform random variables are defined on the interval $[a, b]$. As a result, x_1 and x_2 have a common probability density function given by

$$f(x) = \frac{1}{b - a} \tag{C-3}$$

with the mean (or expected value) [C-2] of

$$\mu = \frac{b + a}{2} \tag{C-4}$$

The variance for this distribution is expressed as

$$\sigma^2 = \frac{(b - a)^2}{12} \tag{C-5}$$

With the use of these formulas, it may be shown that

$$a = 2.0 - 0.4\sqrt{3}$$
$$b = 2.0 + 0.4\sqrt{3} \tag{C-6}$$

C.1 Expected Value of $g(x_1, x_2)$

Based upon this information, a first goal is the compute the expected value of g; defined in general as

$$E(g(x_1, x_2)) = \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} g(x_1, x_2) f(x_1, x_2) dx_1 dx_2 \qquad \text{(C-6)}$$

where f is the joint probability distribution function of x_1 and x_2.[C-2] These two random variables are independent, so the joint probability function is calculated as the product of their individual probability density functions. Hence,

$$f(x_1, x_2) = \frac{1}{(b-a)^2} = \frac{1}{1.92} \qquad \text{(C-7)}$$

Equations (g) and (h) may be used to show that

$$E[g(x_1, x_2)] = \int\limits_a^b \int\limits_a^b \ln(1+x_1^2) \sin(5x_2) \left(\frac{1}{1.92}\right) dx_1 dx_2 \qquad \text{(C-8)}$$

Independence and the product form of g can be used to rewrite (C-8) as

$$E[g(x_1, x_2)] = \frac{1}{1.92} \int\limits_a^b \ln(1+x_1^2) dx_1 \int\limits_a^b \sin(5x_2) dx_2 \qquad \text{(C-9)}$$

The integrals in (C-9) can be evaluated independently, i.e.,

$$\int\limits_a^b \ln(1+x_1^2) dx_1 = \left(x_1 \ln(1+x_1^2) - 2x_1 + 2\tan^{-1}(x_1)\right)\Big|_a^b \qquad \text{(C-10)}$$

$$\int\limits_a^b \sin(5x_2) dx_2 = \frac{1}{5}\left[\cos(5a) - \cos(5b)\right] \qquad \text{(C-11)}$$

With the use of equations (C-10) and (C-11), the expected value of $g(x_1, x_2)$ is calculated as

$$\mu = E[g(x_1, x_2)] = 0.079169 \qquad \text{(C-12)}$$

C.2 Variance of $g(x_1, x_2)$

Calculating the variance of $g(x_1, x_2)$ is substantially more complicated than the expected value computation. The variance σ^2 of a random variable is defined as follows.[C-2]

$$\sigma^2 = E[(X - \mu)^2] = E[X^2] - \mu^2 \qquad \text{(C-13)}$$

To obtain the variance of g, it is necessary to obtain the moment $E[g^2(x_1, x_2)]$. That is,

$$E[g^2(x_1,x_2)] = \frac{1}{(b-a)^2}\int_a^b\int_a^b\left(\ln(1+x_1^2)\right)^2\sin^2(5x_2)\,dx_1\,dx_2 \tag{C-14}$$

Fortunately, the multiple integral above is separable in that

$$E[g^2(x_1,x_2)] = \frac{1}{(b-a)^2}\int_a^b\left(\ln(1+x_1^2)\right)^2 dx_1\int_a^b\sin^2(5x_2)\,dx_2 \tag{C-15}$$

The integral over the random variable x_2 is easily evaluated as

$$\int_a^b\sin^2(5x_2)\,dx_2 = \frac{1}{2}\left[b-a+\frac{1}{10}\left(\sin(10a)-\sin(10b)\right)\right] \tag{C-16}$$

The remaining integral is much more difficult to evaluate. In fact, it cannot be evaluated in terms of elementary functions. With a substantial amount of work, it can be shown that

$$\int_a^b\left(\ln(1+x_1^2)\right)dx_1 = \left(\left(\ln(\sec^2\theta)\right)^2\tan\theta - 4\left(\ln(\sec^2\theta)-2\right)\left(\tan\theta-\theta\right)+8\theta\ln(\cos\theta)\right)\Big|_{\theta_a}^{\theta_b}$$
$$-8\int_{\theta_a}^{\theta_b}\ln(\cos\theta)\,d\theta \tag{C-17}$$

where

$$\begin{aligned}a = \tan\theta_a &\quad\Rightarrow\quad \theta_a = \tan^{-1}(a)\\ b = \tan\theta_b &\quad\Rightarrow\quad \theta_b = \tan^{-1}(b)\end{aligned} \tag{C-18}$$

The final integral in equation (C-17) cannot be evaluated in terms of elementary functions. It requires the use of numerical quadrature or application of the Clausen function CL_2. Appendix E describes the Clausen function, but the core result needed is that

$$\int_0^\theta\ln(\cos\tilde\theta)\,d\tilde\theta = \frac{1}{2}CL_2(\pi-2\theta)-\theta\ln2,\quad 0\le\theta\le\frac{\pi}{2} \tag{C-19}$$

In equation (C-17), the corresponding integral may be written as

$$\int_a^b\ln(\cos\theta)\,d\theta = \int_0^b\ln(\cos\theta)\,d\theta - \int_0^a\ln(\cos\theta)\,d\theta \tag{C-20}$$

Equations (C-19) and (C-20) may be combined to obtain the result

$$\int\limits_{\theta_a}^{\theta_b} \ln(\cos\theta)\,d\theta = \frac{1}{2}\left[\mathrm{CL}_2(\pi - 2\theta_b) - \mathrm{CL}_2(\pi - 2\theta_a)\right] - (\theta_b - \theta_a)\ln 2 \qquad (\text{C-21})$$

Even with good numerical techniques and polynomial series expansions, Clausen functions are challenging to evaluate. For this reason, the definite integral in equation (t) has been evaluated by a variety of techniques. The results are shown in Table C-1. For the numerical approximations, the composite trapezoidal and Simpson's rules are applied. Clausen functions 1 and 2 are described in Appendix E.

Table C-18. Definite Integral of ln (cos θ)

Quadrature Method	Value
Trapezoidal Rule	-0.2211678
Simpson's Rule	-0.2211675
Clausen Formula 1	-0.2206295
Clausen Formula 2	-0.2211681

With the use of equations (C-13), (C-16) and (C-17) with the data in Table 1, variance approximations can be computed for $g(x_1, x_2)$. These results are presented in Table C-2.

Table C-2. Variance Approximations for Random Function g

ln (cos θ) Quadrature Method	Variance	Standard Deviation
Trapezoidal Rule	1.263684	1.124137
Simpson's Rule	1.263683	1.124136
Clausen Formula 1	1.262185	1.123470
Clausen Formula 2	1.263685	1.124137

REFERENCES

C-1. Hosder, S., Walters, R.W. and Balch, M., "Efficient Sampling for Non-Intrusive Polynomial Chaos Applications with Multiple Uncertain Input Variables", AIAA 2007-1939, 48th AIAA/ ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference, 23-26 April 2007, Honolulu, Hawaii.

C-2. Ross, S.M., *Introduction to Probability Models*, 4th Ed., Academic Press, Boston, Massachusetts, 1989.

APPENDIX D

DIRECT STATISTICAL ANALYSIS FOR TEST PROBLEM 4

This test problem involves a model random process that operates on four uniform random variables $x_j = x_j(\xi_j)$, $j = 1,\ldots,4$. Specifically, the process is written

$$f(x_1, x_2, x_3, x_4) = \exp[1.5(x_1 + x_2 + x_3 + x_4)] \tag{D-1}$$

These variables, in turn, rely upon the 4 standard uniform variables ξ_j, $\xi_j \in [-1,1]$. For the random variables, x_j, $j = 1,\ldots,4$, the mean value is 0.4 and the coefficient of variation is 0.4.[D-1] From this information, it can be shown that the domain of x_j is

$$x_j \in [a,b] = [0.4 - 0.08\sqrt{12}, 0.4 + 0.08\sqrt{12}] \tag{D-2}$$

Since (D-1) operates on four independent uniform random variables, the joint probability density function is written as

$$w(x_1, x_2, x_3, x_4) = \frac{1}{(b-a)^4} \tag{D-3}$$

The expected value of the random process is then computed as

$$E(f) = \int_a^b \int_a^b \int_a^b \int_a^b \exp[1.5(x_1 + x_2 + x_3 + x_4)] \frac{1}{(b-a)^4} dx_1 \, dx_2 \, dx_3 \, dx_4 \tag{D-4}$$

$$E(f) = \frac{1}{(b-a)^4} \int_a^b \exp(1.5x_1)dx_1 \int_a^b \exp(1.5x_2)dx_2 \int_a^b \exp(1.5x_3)dx_3 \int_a^b \exp(1.5x_4)dx_4 \tag{D-5}$$

The recurring integral appearing in (D-5) is easily calculated as

$$\int_a^b \exp(1.5x)\,dx = \frac{\exp(1.5x)}{1.5}\Big|_a^b = \frac{2}{3}[\exp(1.5b) - \exp(1.5a)] \tag{D-6}$$

with a and b given by (D-2). As a result, the expected value becomes

$$E(f) = \left[\frac{2}{3(b-a)}(\exp(1.5b) - \exp(1.5a)) \right]^4 = 12.3609 \tag{D-7}$$

The second moment of this random process may be calculated in the same way after noting that

$$f^2(x_1, x_2, x_3, x_4) = \left[\exp(1.5(x_1 + x_2 + x_3 + x_4))\right]^2 = \exp[3(x_1 + x_2 + x_3 + x_4)] \qquad \text{(D-8)}$$

The associated integral for $E(f^2)$ has the same form as (D-5); thus, with

$$\int_a^b \exp(3x)\,dx = \frac{1}{3}\left[\exp(3b) - \exp(3a)\right] \qquad \text{(D-9)}$$

we have that

$$E(f^2) = \left[\frac{1}{3(b-a)}\left(\exp(3b) - \exp(3a)\right)\right] \qquad \text{(D-10)}$$

Using the definitions of variance and standard deviation, the standard deviation is calculated as

$$\sigma = 6.1556 \qquad \text{(D-11)}$$

REFERENCES

D-1. Hosder, S., Walters, R.W. and Balch, M., "Efficient Sampling for Non-Intrusive Polynomial Chaos Applications with Multiple Uncertain Input Variables", AIAA 2007-1939, 48th AIAA/ ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference, 23-26 April 2007, Honolulu, Hawaii.

Distribution A

APPENDIX E

CLAUSEN'S FUNCTION

In association with the polylogarithm, polygamma and Riemann Zeta functions, the Clausen function has applications in physics, such as in the field of electrodynamics.[E-1] As is indicated by this report, it also has uses in probability modeling. Clausen's function is defined as follows.

$$CL_2(\theta) = -\int_0^\theta \ln\left|2\sin\left(\frac{x}{2}\right)\right|dx \tag{E-1}$$

A theoretical series expansion also exists for this function, i.e,

$$CL_2(\theta) = \sum_{k=1}^\infty \frac{\sin(k\theta)}{k^2} \tag{E-2}$$

This infinite series is slowly convergent and generally not used for calculations. Instead, series based upon Chebyshev polynomials are often recommended for generating the Clausen functions.[E-2,E-3] Although these methods are accurate, they are computationally complicated and still involve the use of infinite series. These difficulties motivate the use of numerical quadrature techniques and approximate functional forms.

The Clausen integral (E-1) can be evaluated by the use of basic numerical integration techniques such as the composite forms of the Trapezoidal and Simpson's rules.[E-4] To justify the use of quadrature on (E-1), it is necessary to show that the integrand is finite at the lower limit of integration. At first glance, the sine function is zero at zero, so the natural logarithm at this point would seem to tend to minus infinity. This potential difficulty requires more in-depth analysis. By applying the asymptotic approximation for the sine function of small arguments, we have that

$$\sin\left(\frac{x}{2}\right) \approx \frac{x}{2} \quad \Rightarrow \quad \ln\left|\sin\left(\frac{x}{2}\right)\right| \approx \ln\left(\frac{x}{2}\right) \approx \ln(x) \tag{E-3}$$

The absolute value bars have been eliminated from (E-3) since x is confined to the domain $[0, \pi]$. With this approximation, we can estimate the Clausen integral as

$$\int_0^\theta \ln\left|2\sin\left(\frac{x}{2}\right)\right|dx \approx \int_0^\theta \ln(x)\,dx \approx \left(x\ln(x) - x\right)\big|_0^\theta \tag{E-4}$$

If this result is finite in the limit as $x \to 0$, then the Clausen integral is finite and can be approximated by quadrature. This limit is evaluated as follows.
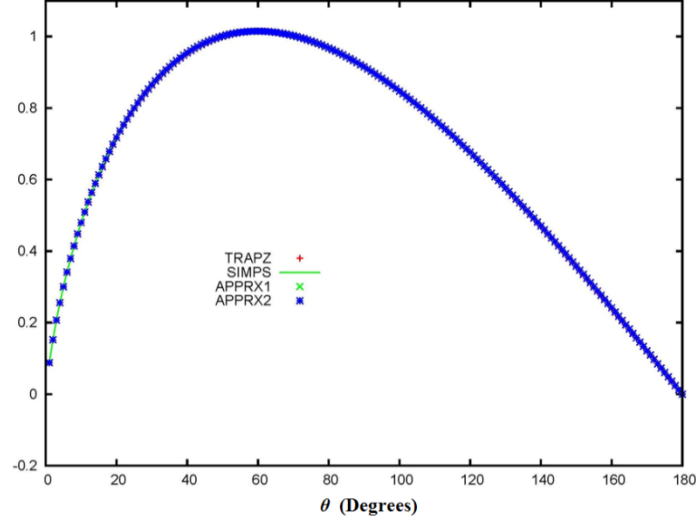
Figure E-1. Approximate values of the Clausen function versus an angular argument

$$\lim_{x \to 0} x \ln(x) = \lim_{x \to 0} \frac{\ln(x)}{1/x} = \lim_{x \to 0} \left(\frac{1/x}{-1/x^2} \right) = \lim_{x \to 0} (-x) = 0 \tag{E-5}$$

L'Hopital's rule has been employed in obtaining this result, so the Clausen integral is finite and may be evaluated by use of the composite Trapezoidal and Simpson rules. Alternatively, formula approximations may be used to evaluate the Clausen function.

For comparison, there are two approximate formulas for the Clausen function.[E-5] The simpler formula is given as

$$CL_2(\theta) = -\theta \ln\left(\theta/2\right) + \theta/24 \left(\pi^2 - \theta^2\right) - \left(3/2 - 2\ln 2\right)\sin\theta + \left(\ln 2 - 11/16\right)\sin 2\theta \tag{E-6}$$

where $0 \le \theta \le \pi$. The second formula, regarded to be of higher accuracy, may be written as

$$CL_2(\theta) = -\theta \ln \sin\left(\theta/2\right) + \theta/2880 \left(\pi^2 - \theta^2\right)\left(120 - 7\pi^2 + 3\theta^2\right) + \left(2\ln 2 - 5/4\right)\sin\theta$$
$$- \left(89/128 - \ln 2\right)\sin 2\theta + \left(2/3 \ln 2 - 449/972\right)\sin 3\theta \tag{E-7}$$
$$- \left(4259/12288 - 1/2 \ln 2\right)\sin 4\theta + \left(2/5 \ln 2 - 10397/37500\right)\sin 5\theta$$

where $0 \le \theta \le \pi$. A relative error of 0.63% is quoted for (E-6) while a relative error of 0.003% is similarly quoted for (E-7).[E-3] These error estimates must be qualified because the theory restricts the argument θ to a rational multiple of π where a rational argument is the ratio of two integers. The meaning in this case is that (E-6) and (E-7) are not valid, in the strictest sense, for irrational multiples of π. It is more difficult to quantify accuracy in this case. Still, these formulas seem suitable enough for performing comparison calculations. A plot of the Clausen function

41

evaluated by trapezoidal rule (TRAPZ), Simpson's rule (SIMPS), formula (E-6) (APPRX1) and formula (E-7) (APPRX2) are shown in Figure (E-1).

In Appendix C, the computation of variance requires evaluating the integral of the logarithmic cosine, i.e.,

$$\int_0^\theta \ln(\cos x)\, dx \qquad\qquad (E\text{-}8)$$

This integral can be evaluated as follows. We begin with the Clausen integral, i.e.,

$$CL_2(\theta) = -\int_0^\theta \ln\left|2\sin\left(\frac{x}{2}\right)\right| dx \qquad\qquad (E\text{-}9)$$

By using the transformation of variables $x = 2y$ along with the trigonometric identity

$$\sin y = \sin\left(\frac{y}{2} + \frac{y}{2}\right) = 2\sin\left(\frac{y}{2}\right)\cos\left(\frac{y}{2}\right) \qquad\qquad (E\text{-}10)$$

By substituting (E-10) into (E-9) and by applying a property of the logarithm,

$$CL_2(\theta) = -2\int_0^{\theta/2} \ln\left|2\sin\left(\frac{y}{2}\right)\right| dy - 2\int_0^{\theta/2} \ln\left|2\cos\left(\frac{y}{2}\right)\right| dy \qquad\qquad (E\text{-}11)$$

Equation (E-9) easily demonstrates that

$$\frac{1}{2}CL_2(\theta) = -CL_2(\theta/2) - \int_0^{\theta/2} \ln\left|2\cos\left(\frac{y}{2}\right)\right| dy \qquad\qquad (E\text{-}12)$$

With the change of variables $y = 2x$, we have that

$$\int_0^{\theta/4} \ln\left|2\cos x\right| dx = -\frac{1}{4}CL_2(\theta) - \frac{1}{2}CL_2(\theta/2) \qquad\qquad (E\text{-}13)$$

By replacing θ with 4θ, we obtain

$$\int_0^\theta \ln\left|2\cos x\right| dx = -\frac{1}{4}CL_2(4\theta) - \frac{1}{2}CL_2(2\theta) \qquad\qquad (E\text{-}14)$$

The Clausen identity

$$CL_2(2\theta) = 2CL_2(\theta) - 2CL_2(\pi - 2\theta) \qquad \text{(E-15)}$$

may be repeatedly applied to obtain

$$\int_0^\theta \ln|2\cos x|\,dx = \frac{1}{2}CL_2(\pi - 2\theta) \qquad \text{(E-16)}$$

Hence,

$$\int_0^\theta \ln|\cos x|\,dx = \frac{1}{2}CL_2(\pi - 2\theta) - \theta\ln 2 \qquad \text{(E-17)}$$

The notation CL_2 denotes a Clausen function of the second order. Although this second order function is more commonly used, higher order Clausen function, e.g., CL_4, CL_6, exist.[E-3] These functions are evaluated from series of orthogonal polynomials. This numerical procedure is more complicated than either of the quadrature rules mentioned earlier or the formulas above. The methods used to compute the CL_2 create curves that map closely together. Hence, we have confidence in applying quadrature formulas for evaluating Clausen's functions.

REFERENCES

E-1. Lewin, L., Ed., *Structural Properties of Polylogarithms*, American Mathematical Society, Providence, Rhode Island, 1991.

E-2. Wood, V.E., "Efficient calculation of Clausen's integral", *Mathematics of Computation*, Vol. 22, 1968, pp. 883-884.

E-3. Wu, J., Zhang, X. and Liu, D., "An efficient calculation of the Clausen functions $CL_2(\theta)$ $(n \geq 2)$", *BIT Numerical Mathematics*, Vol. 50, No. 1, 2010, pp. 193-206.

E-4. Burden, R.L., Faires, J.D. and Reynolds, A.C., *Numerical Analysis*, 2nd Ed., Prindle, Weber & Schmidt, Boston, Massachusetts, 1981.

E-5. Grosjean, C.C., "Formulae concerning the computation of the Clausen integral $CL_2(\theta)$", *Journal of Computational and Applied Mathematics*, Vol. 11, 1984, pp. 331-342.

LIST OF SYMBOLS, ABBREVIATIONS AND ACRONYMS

CFD......................Computational Fluid Dynamics
E..........................Error
H_n........................Hermite polynomial
LESLIE3D ....Large Eddy Simulation with Linear Eddy Modeling in 3 Dimensions
L_n..........................Legendre polynomial
PC........................Polynomial chaos
w..........................Probability density function
α ....Stochastic or random process
α_j..........................Expansion coefficients
ξ_n ....Random variable
$\vec{\xi}$ ....Vector of random variables
Ψ_n ....Orthogonal polynomial
θ ....Random event
Ω ....Event space

DISTRIBUTION LIST
AFRL-RW-EG-TR-2015-108

*Defense Technical Info Center   AFRL/RWML (1)
8725 John J. Kingman Rd Ste 0944   AFRL/RWORR (STINFO Office) (1)
Fort Belvoir VA 22060-6218